Trimethyl phosphate

512-56-1 | DTXSID1021403

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.414

Global applicability domain: Inside

Local applicability domain index: 4.58e-01

Confidence level: 4.91e-01

Nearest Neighbors from the Training Set

Image not found
Trimethyl phosphate
Measured: -0.650
Predicted: -0.414

Image not found
Diethyl sulfate
Measured: 1.14
Predicted: 6.95e-01

Image not found
cis-Mevinphos
Measured: 0.13
Predicted: 9.28e-02

Image not found
Diethyl propanedioate
Measured: 0.96
Predicted: 8.73e-01